

09779331

Welcome to STN International! Enter x:x

LOGINID:ssspta1202sxq

PASSWORD:

TERMINAL (ENTER 1, 2, 3, OR ?):2

* * * * * Welcome to STN International * * * * *

NEWS 1 Web Page URLs for STN Seminar Schedule - N. America
NEWS 2 Apr 08 "Ask CAS" for self-help around the clock
NEWS 3 Apr 09 BEILSTEIN: Reload and Implementation of a New Subject Area
NEWS 4 Apr 09 ZDB will be removed from STN
NEWS 5 Apr 19 US Patent Applications available in IFICDB, IFIPAT, and IFIUDB
NEWS 6 Apr 22 Records from IP.com available in CAPLUS, HCAPLUS, and ZCAPLUS
NEWS 7 Apr 22 BIOSIS Gene Names now available in TOXCENTER
NEWS 8 Apr 22 Federal Research in Progress (FEDRIP) now available
NEWS 9 Jun 03 New e-mail delivery for search results now available
NEWS 10 Jun 10 MEDLINE Reload
NEWS 11 Jun 10 PCTFULL has been reloaded
NEWS 12 Jul 02 FOREGE no longer contains STANDARDS file segment
NEWS 13 Jul 22 USAN to be reloaded July 28, 2002;
saved answer sets no longer valid
NEWS 14 Jul 29 Enhanced polymer searching in REGISTRY
NEWS 15 Jul 30 NETFIRST to be removed from STN
NEWS 16 Aug 08 CANCERLIT reload
NEWS 17 Aug 08 PHARMAMarketLetter(PHARMAML) - new on STN
NEWS 18 Aug 08 NTIS has been reloaded and enhanced
NEWS 19 Aug 19 Aquatic Toxicity Information Retrieval (AQUIRE)
now available on STN
NEWS 20 Aug 19 IFIPAT, IFICDB, and IFIUDB have been reloaded
NEWS 21 Aug 19 The MEDLINE file segment of TOXCENTER has been reloaded
NEWS 22 Aug 26 Sequence searching in REGISTRY enhanced
NEWS 23 Sep 03 JAPIO has been reloaded and enhanced
NEWS 24 Sep 16 Experimental properties added to the REGISTRY file
NEWS 25 Sep 16 Indexing added to some pre-1967 records in CA/CAPLUS
NEWS 26 Sep 16 CA Section Thesaurus available in CAPLUS and CA
NEWS 27 Oct 01 CASREACT Enriched with Reactions from 1907 to 1985
NEWS 28 Oct 21 EVENTLINE has been reloaded
NEWS 29 Oct 24 BEILSTEIN adds new search fields
NEWS 30 Oct 24 Nutraceuticals International (NUTRACEUT) now available on STN
NEWS 31 Oct 25 MEDLINE SDI run of October 8, 2002
NEWS 32 Nov 18 DKILIT has been renamed APOLLIT
NEWS 33 Nov 25 More calculated properties added to REGISTRY

NEWS EXPRESS October 14 CURRENT WINDOWS VERSION IS V6.01,
CURRENT MACINTOSH VERSION IS V6.0a(ENG) AND V6.0Ja(JP),
AND CURRENT DISCOVER FILE IS DATED 01 OCTOBER 2002
NEWS HOURS STN Operating Hours Plus Help Desk Availability
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Enter NEWS followed by the item number or name to see news on that

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specific topic.

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* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 16:59:29 ON 30 NOV 2002

=> ile caplus

ILE IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.
For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

=> file caplus

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.21	0.21

FILE 'CAPLUS' ENTERED AT 16:59:42 ON 30 NOV 2002

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FILE COVERS 1907 - 30 Nov 2002 VOL 137 ISS 23

FILE LAST UPDATED: 29 Nov 2002 (20021129/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

=> s 2-hydroxypropyl estradiol

7534268 2

31476 HYDROXYPROPYL

65277 ESTRADIOL

L1 1 2-HYDROXYPROPYL ESTRADIOL

11/30/02

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L2 65277 ESTRADIOL

=> s l1 and 2-substituted

7534268 2

414275 SUBSTITUTED

11120 2-SUBSTITUTED

(2(W)SUBSTITUTED)

L3 0 L1 AND 2-SUBSTITUTED

=> file reg

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

13.24

13.45

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

SINCE FILE

TOTAL

ENTRY

SESSION

CA SUBSCRIBER PRICE

-0.62

-0.62

FILE 'REGISTRY' ENTERED AT 17:01:46 ON 30 NOV 2002

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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 29 NOV 2002 HIGHEST RN 474744-87-1

DICTIONARY FILE UPDATES: 29 NOV 2002 HIGHEST RN 474744-87-1

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> s 2-hydroxypropyl estradiol

14553906 2

74965 HYDROXYPROPYL

1212 ESTRADIOL

L4 0 2-HYDROXYPROPYL ESTRADIOL

(2(W)HYDROXYPROPYL(W)ESTRADIOL)

=> s 2-hydroxymethyl estradiol

14553906 2

203646 HYDROXYMETHYL

1212 ESTRADIOL

L5 0 2-HYDROXYMETHYL ESTRADIOL

(2(W)HYDROXYMETHYL(W)ESTRADIOL)

=> 2-methoxymethyl estradiol

2-METHOXYMETHYL IS NOT A RECOGNIZED COMMAND

The previous command name entered was not recognized by the system.

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For a list of commands available to you in the current file, enter
"HELP COMMANDS" at an arrow prompt (=>).

```
=> s 2-methoxymethyl estradiol
      14553906 2
          90600 METHOXYMETHYL
          1212 ESTRADIOL
L6      0 2-METHOXYMETHYL ESTRADIOL
          (2(W)METHOXYMETHYL(W)ESTRADIOL)
```

```
=> file caplus
COST IN U.S. DOLLARS                SINCE FILE      TOTAL
                                     ENTRY      SESSION
FULL ESTIMATED COST                37.52      50.97

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)  SINCE FILE      TOTAL
                                               ENTRY      SESSION
CA SUBSCRIBER PRICE                  0.00      -0.62
```

FILE 'CAPLUS' ENTERED AT 17:04:09 ON 30 NOV 2002
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FILE COVERS 1907 - 30 Nov 2002 VOL 137 ISS 23
FILE LAST UPDATED: 29 Nov 2002 (20021129/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

CAS roles have been modified effective December 16, 2001. Please check your SDI profiles to see if they need to be revised. For information on CAS roles, enter HELP ROLES at an arrow prompt or use the CAS Roles thesaurus (/RL field) in this file.

```
=> s 16-substituted estradiol
      683467 16
          414275 SUBSTITUTED
          65277 ESTRADIOL
L7      1 16-SUBSTITUTED ESTRADIOL
          (16(W)SUBSTITUTED(W)ESTRADIOL)
```

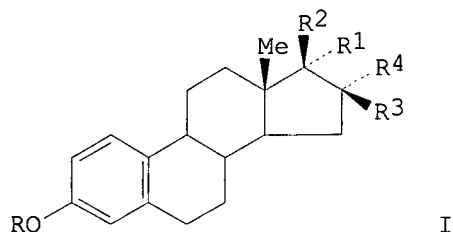
```
=> d 17 ibib hitstr abs
```

```
L7  ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2002 ACS
ACCESSION NUMBER:      1985:46179  CAPLUS
DOCUMENT NUMBER:       102:46179
```

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TITLE: Syntheses of **16-substituted estradiol** derivatives
AUTHOR(S): Tong, Zhengshou; Gan, Guizhi; Li, Lu
CORPORATE SOURCE: Acad. Mil. Med. Sci., Peop. Rep. China
SOURCE: Yiyao Gongye (1984), (8), 14-17
CODEN: YIGODN; ISSN: 0255-7223
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
GI



AB The title compds. I [R, R1, R2, R3, R4 = H, H, OH, H, OH; H, H, OH, OH, H; H, H, OH, OH, C.tplbond.CH; H, H, OCMe2O (R2R3), C.tplbond.CH; H, H, OCMe2O (R2R3), H; Ac, O (R1R4), OAc (R2), H (R3); Ac, O (R1R2), H, OAc; H, O (R1R2), H, OH; H, H, OH, O (R3R4); Ac, H, OAc, O (R3R4)] were prepd. from estrone by conventional methods.

=> s 2-substituted estradiol
7534268 2
414275 SUBSTITUTED
65277 ESTRADIOL

L8 5 2-SUBSTITUTED ESTRADIOL
(2 (W) SUBSTITUTED (W) ESTRADIOL)

=> d l8 ibib hitstr abs

L8 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 2002:157582 CAPLUS
DOCUMENT NUMBER: 136:200348
TITLE: Preparation of **2-substituted estradiol** derivatives for inhibiting superoxide dismutase
INVENTOR(S): Potter, Barry Victor Lloyd; Reed, Michael John; Packham, Graham Keith
PATENT ASSIGNEE(S): Sterix Limited, UK
SOURCE: PCT Int. Appl., 71 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 4
PATENT INFORMATION:

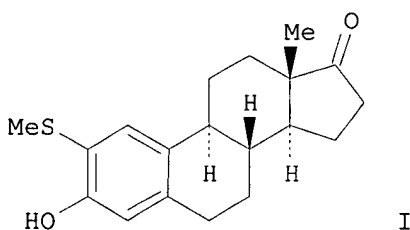
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002015910	A1	20020228	WO 2001-GB3715	20010817
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN,				

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CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH,
GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL,
PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG,
US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY,
DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF,
BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG

AU 2001079955 A5 20020304 AU 2001-79955 20010817
PRIORITY APPLN. INFO.: GB 2000-20498 A 20000818
GB 2001-13921 A 20010607
WO 2001-GB3715 W 20010817

OTHER SOURCE(S): MARPAT 136:200348
GI



AB Title compds. R1XK (X is a ring having at least 4 atoms in the ring; K is a hydrocarbyl group; R1 is a halo, or a group of the formula -L1-Z-R1', L1 is an optional linker group, Z is O or S and R1' is a hydrocarbyl group or H; with the proviso that the compd. is other than 2-methoxy-17.beta.-estradiol, 2-methoxyoestrone and 2-hydroxyestradiol) were prep'd. to inhibit superoxide dismutase (SOD) or for use in the therapy of a condition or disease assoc'd. with SOD. Thus oestrone was converted to the ethylene ketal and then to the methoxymethyl ether deriv., which reacted with di-Me disulfide followed by deprotection to give 2-(methylthio)-1,3,5(10)-estratrien-3-ol (I). The superoxide dismutase inhibiting IC50 of I was 21 +/- .5 .mu.M.

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d 18 1-5 ibib hitstr abs

L8 ANSWER 1 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 2002:157582 CAPLUS

DOCUMENT NUMBER: 136:200348

TITLE: Preparation of **2-substituted estradiol** derivatives for inhibiting superoxide dismutase

INVENTOR(S): Potter, Barry Victor Lloyd; Reed, Michael John; Packham, Graham Keith

PATENT ASSIGNEE(S): Sterix Limited, UK

SOURCE: PCT Int. Appl., 71 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent

LANGUAGE: English

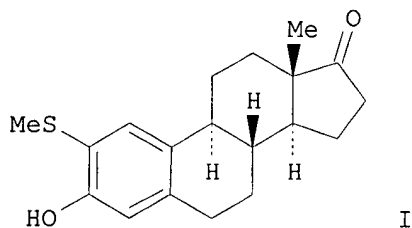
FAMILY ACC. NUM. COUNT: 4

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PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002015910	A1	20020228	WO 2001-GB3715	20010817
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2001079955	A5	20020304	AU 2001-79955	20010817
PRIORITY APPLN. INFO.:			GB 2000-20498	A 20000818
			GB 2001-13921	A 20010607
			WO 2001-GB3715	W 20010817
OTHER SOURCE(S):			MARPAT 136:200348	
GI				



AB Title compds. R1XK (X is a ring having at least 4 atoms in the ring; K is a hydrocarbyl group; R1 is a halo, or a group of the formula -L1-Z-R1', L1 is an optional linker group, Z is O or S and R1' is a hydrocarbyl group or H; with the proviso that the compd. is other than 2-methoxy-17.β-estradiol, 2-methoxyoestrone and 2-hydroxyestradiol) were prepd. to inhibit superoxide dismutase (SOD) or for use in the therapy of a condition or disease assocd. with SOD. Thus oestrone was converted to the ethylene ketal and then to the methoxymethyl ether deriv., which reacted with di-Me disulfide followed by deprotection to give 2-(methylthio)-1,3,5(10)-estratrien-3-ol (I). The superoxide dismutase inhibiting IC50 of I was 21 ± 0.5 μM.

REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L8 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1997:321168 CAPLUS

DOCUMENT NUMBER: 127:28213

TITLE: Technetium and rhenium labeled steroids. Part 1. First synthesis of "3+1" mixed-ligand oxorhenium(V) complexes bearing a pendant estradiol moiety

AUTHOR(S): Wust, F.; Spies, H.; Scheller, D.; Machill, S.

CORPORATE SOURCE: Inst. Bioinorganic Radiopharmaceutical Chemistry, Research Center Rossendorf Inc., Dresden, D-01314, Germany

SOURCE: Forschungszentrum Rossendorf e.V., [Bericht] FZR (1997

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), FZR-165, 86-90

CODEN: FRBFEU

DOCUMENT TYPE:

Report

LANGUAGE:

English

AB First investigations on the chem. of estradiol-Re complexes, starting from easily available **2-substituted estradiol** derivs. are described. The reaction sequence of 2-thiomethyl-estra-1,3,5(10)-triene-3,17.beta.-diol (I) is given. The "3+1" mixed-ligand Re complexes (3-thiapentane-1,5-dithiolato)(3,17.beta.-estradiol-2-thiomethylato)oxorhenium(V) and (3-oxapentane-1,5-dithiolato)(3,17.beta.-estradiol-2-thiomethylato)oxorhenium(V) are prepd. by reaction of the monothiol I with Re precursors. ¹³C NMR spectroscopy was used to elucidate the structure of the prepd. steroid compds.

L8 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1995:139039 CAPLUS

DOCUMENT NUMBER: 122:187855

TITLE: Synthesis and uterotrophic activity of 2-**substituted estradiol** and ring A fused pyranone and furanone derivatives

AUTHOR(S): Ismail, Khadiga A.; El-Medany, Azza

CORPORATE SOURCE: Faculty of Pharmacy, University of Alexandria, Egypt

SOURCE: Alexandria Journal of Pharmaceutical Sciences (1994), 8(2), 95-9

CODEN: AJPSES; ISSN: 1110-1792

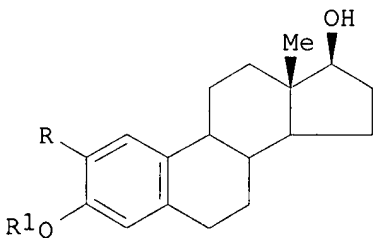
DOCUMENT TYPE:

Journal

LANGUAGE:

English

GI



I

AB New modified estradiol analogs I [R = R2COCH2CO, R2COCHBrCO, R1 = H, R2 = Me, Ph; RR1 = COCBr:CR2, COCH(COR2)] have been synthesized and examd. as potential estrogens. Uterine wt. assays in rats have shown that all these compds. produced a moderate increase in uterine wt.

L8 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1994:183184 CAPLUS

DOCUMENT NUMBER: 120:183184

TITLE: Synthesis, binding affinities and uterotrophic activity of some 2-**substituted estradiol** and ring-A-fused pyrone derivatives

AUTHOR(S): Omar, A. M. M. E.; Ahmed, I. C.; AboulWafa, O. M.; Hassan, A. M.; Ismail, K. A.; El-Din, M. M. M.; Mansour, N. A.

CORPORATE SOURCE: Dep. Pharmaceut. Chem., Fac. Pharm., Alexandria, Egypt

SOURCE: European Journal of Medicinal Chemistry (1994), 29(1),

25-32

CODEN: EJMCA5; ISSN: 0223-5234

DOCUMENT TYPE:

Journal

LANGUAGE:

English

AB A series of estradiol analogs has been synthesized and examd. as potential estrogens. Nuclear modifications included a variety of substituents at the 2 position of estradiol, which was previously thought to be inhibitory for activity, and inclusion of the 3-phenolic hydroxyl group in a .gamma.-pyrone and 3'-formylchromone rings fused to ring A of estradiol. The estrogen relative binding affinities and in vivo assays for uterotrophic activity in rats showed that all the tested compds. were capable of displacing [3H]E2 from the estrogen receptor sites by different degrees. The highest inhibition of [3H]E2 binding (78%) to the estrogen receptor was displayed by 2-acetylestestradiol which was also a potent uterotrophic agent. Omission of the free 3-hydroxyl functionality by inclusion in a .gamma.-pyrone ring produced a chromone deriv. that was capable of inhibiting [3H]E2 binding by 60% and displayed a uterotrophic response of 97%. Further nuclear modification by introduction of thiosemicarbazone moieties decreased the uterotrophic activity, the highest activity being elicited by the p-bromophenyl thiosemicarbazone deriv. The diketone 2-benzoylacetylestestradiol 17.beta.-acetate, 2-(3'-benzylideneacetyl)estradiol and 2-[3'-(3-anisylidene)acetyl]estradiol exhibited high inhibition of binding affinity while eliciting .apprxeq. 50% the uterotrophic activity of estradiol.

L8 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2002 ACS

ACCESSION NUMBER: 1992:255863 CAPLUS

DOCUMENT NUMBER: 116:255863

TITLE: Synthesis and evaluation for uterotropic and antiimplantation activities of 2-substituted estradiol derivatives

AUTHOR(S): AboulWafa, Omaima M.; El-Din, Mahmoud M. Mohy; Omar, A. Mohsen M. E.

CORPORATE SOURCE: Fac. Pharm., Univ. Alexandria, Alexandria, Egypt

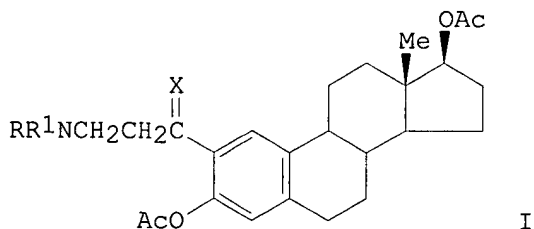
SOURCE: Steroids (1992), 57(4), 199-204

CODEN: STEDAM; ISSN: 0039-128X

DOCUMENT TYPE: Journal

LANGUAGE: English

GI



AB Two novel series of 2-substituted estradiol derivs. I [R = R1 = Me, Et; NRR1 = piperidino, morpholino; X = O, NNHC(:X1)NH2; X1 = O, S) have been synthesized and evaluated for uterotropic and antiimplantation activities. Among the compds. tested in the rat 2-acetylestestradiol 17.beta.-acetate and I (R = R1 = Me, Et, NRR1 = piperidino, X = O; R = R1 = Et, NRR1 = morpholino, X = NNHC(:X1)NH2) displayed

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estrogenic activity. At dosages of 4 .mu.g/rat/day, none of the tested compds. elicited antiimplantation activity. All compds. shared a similar characteristic, nuclear substitution at the C-2 position of the steroid nucleus, a property previously thought to be markedly inhibitory for estrogenic activity.

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Welcome to STN International! Enter x:x

LOGINID:ssspta1202sxq

PASSWORD:

* * * * * RECONNECTED TO STN INTERNATIONAL * * * * *
SESSION RESUMED IN FILE 'CAPLUS' AT 17:11:15 ON 30 NOV 2002
FILE 'CAPLUS' ENTERED AT 17:11:15 ON 30 NOV 2002
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COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	33.05	84.02
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-4.34	-4.96

=> file reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	33.44	84.41
DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	-4.34	-4.96

FILE 'REGISTRY' ENTERED AT 17:11:37 ON 30 NOV 2002
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STRUCTURE FILE UPDATES: 29 NOV 2002 HIGHEST RN 474744-87-1
DICTIONARY FILE UPDATES: 29 NOV 2002 HIGHEST RN 474744-87-1

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
<http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf>

=> s methoxyestradiol
L12 22 METHOXYESTRADIOL

=> d 1-3

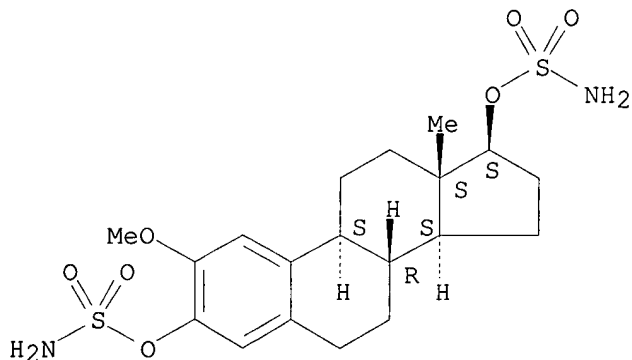
L12 ANSWER 1 OF 22 REGISTRY COPYRIGHT 2002 ACS

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RN 401600-86-0 REGISTRY
CN Estradiol, 17-((2-methoxy-1,3,5-triene-3-yl)oxy)-, 2-methoxy-, disulfamate, (17.β.)-(9CI) (CA INDEX NAME)
OTHER NAMES:
CN **2-Methoxyestradiol disulfamate**
FS STEREOSEARCH
MF C19 H28 N2 O7 S2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

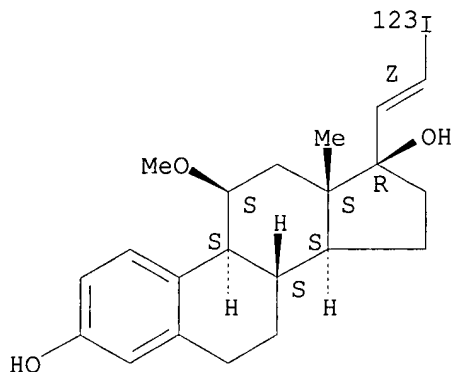
2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L12 ANSWER 2 OF 22 REGISTRY COPYRIGHT 2002 ACS
RN 177159-11-4 REGISTRY
CN 19-Norpregna-1,3,5(10),20-tetraene-3,17-diol, 21-(iodo-123I)-11-methoxy-, (11.β.,17.α.,20Z)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN **(Z)-17.α.-[123I]-2-(Iodovinyl)-11.β.-methoxyestradiol**
CN (Z)-[123I]MIVE
FS STEREOSEARCH
DR 142155-00-8
MF C21 H27 I O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.

Double bond geometry as described by E or Z.

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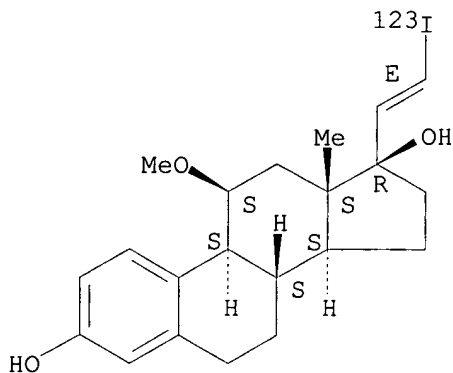
5 REFERENCES IN FILE CA (1962 TO DATE)
5 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L12 ANSWER 3 OF 22 REGISTRY COPYRIGHT 2002 ACS
RN 177159-10-3 REGISTRY
CN 19-Norpregna-1,3,5(10),20-tetraene-3,17-diol, 21-(iodo-123I)-11-methoxy-,
(11.beta.,17.alpha.,20E)- (9CI) (CA INDEX NAME)

OTHER NAMES:

CN **(E)-17.alpha.-[123I]-2-(Iodovinyl)-11.beta.-methoxyestradiol**
CN (E)-[123I]MIVE
FS STEREOSEARCH
DR 142154-99-2
MF C21 H27 I O3
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.
Double bond geometry as shown.



3 REFERENCES IN FILE CA (1962 TO DATE)
3 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> s 2-methoxyestradiol
14553906 2
22 METHOXYESTRADIOL
L13 10 2-METHOXYESTRADIOL
(2(W)METHOXYESTRADIOL)

11/30/02

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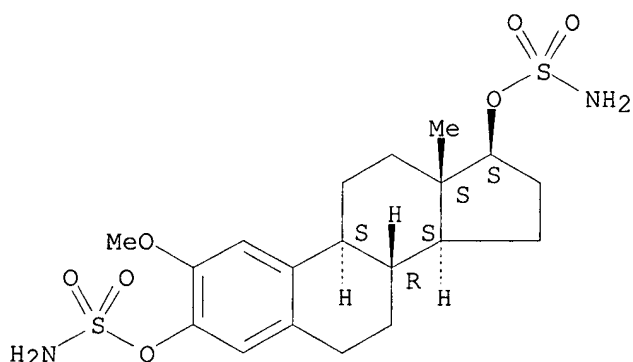
=> d 113 1-2

L13 ANSWER 1 OF 10 REGISTRY COPYRIGHT 2002 ACS
RN 401600-86-0 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 2-methoxy-, disulfamate, (17.beta.)-
(9CI) (CA INDEX NAME)

OTHER NAMES:

CN **2-Methoxyestradiol disulfamate**
FS STEREOSEARCH
MF C19 H28 N2 O7 S2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

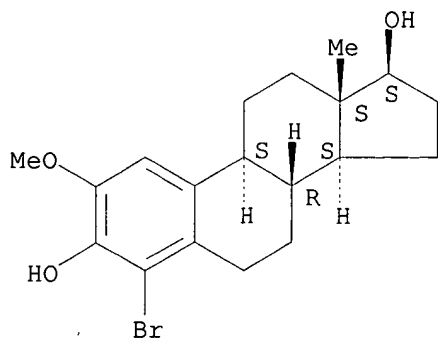
L13 ANSWER 2 OF 10 REGISTRY COPYRIGHT 2002 ACS
RN 97515-50-9 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 4-bromo-2-methoxy-, (17.beta.)- (9CI)
(CA INDEX NAME)

OTHER NAMES:

CN **4-Bromo-2-methoxyestradiol**
FS STEREOSEARCH
MF C19 H25 Br O3
SR CA
LC STN Files: BEILSTEIN*, CA, CAPLUS, CASREACT, TOXCENTER
(*File contains numerically searchable property data)

Absolute stereochemistry.

09779331



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> s 2-ethoxyestradiol
14553906 2
2 ETHOXYESTRADIOL
L14 2 2-ETHOXYESTRADIOL
(2(W)ETHOXYESTRADIOL)

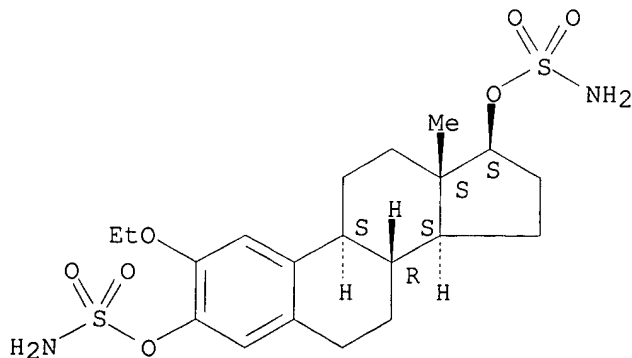
=> d l14 1-2

L14 ANSWER 1 OF 2 REGISTRY COPYRIGHT 2002 ACS
RN 401600-87-1 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 2-ethoxy-, disulfamate, (17.beta.)-
(9CI) (CA INDEX NAME)

OTHER NAMES:

CN **2-Ethoxyestradiol disulfamate**
FS STEREOSEARCH
MF C20 H30 N2 O7 S2
SR CA
LC STN Files: CA, CAPLUS, TOXCENTER

Absolute stereochemistry.



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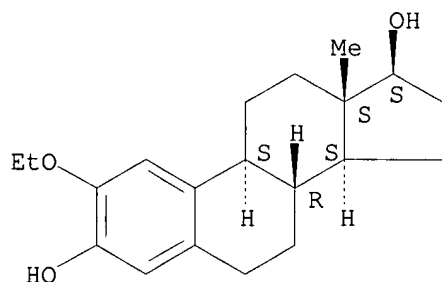
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PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

2 REFERENCES IN FILE CA (1962 TO DATE)
2 REFERENCES IN FILE CAPLUS (1962 TO DATE)

L14 ANSWER 2 OF 2 REGISTRY COPYRIGHT 2002 ACS
RN 165619-07-8 REGISTRY
CN Estra-1,3,5(10)-triene-3,17-diol, 2-ethoxy-, (17.beta.)- (9CI) (CA INDEX
NAME)
OTHER NAMES:
CN **2-Ethoxyestradiol**
CN NSC 671043
FS STEREOSEARCH
MF C20 H28 O3
SR CA
LC STN Files: BIOSIS, CA, CAPLUS, TOXCENTER, USPATFULL

Absolute stereochemistry. Rotation (+).



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

13 REFERENCES IN FILE CA (1962 TO DATE)
13 REFERENCES IN FILE CAPLUS (1962 TO DATE)

=> s 2-alkoxyestradiol
14553906 2
0 ALKOXYESTRADIOL
L15 0 2-ALKOXYESTRADIOL
(2(W) ALKOXYESTRADIOL)

=> logoff
ALL L# QUERIES AND ANSWER SETS ARE DELETED AT LOGOFF

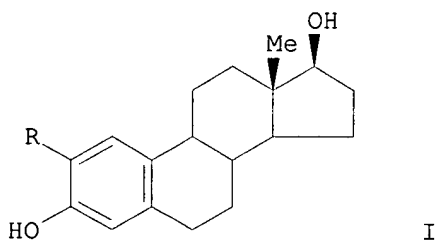
11/30/02

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(2(W) HYDROXYPROPYL(W) ESTRADIOL)

=> d l1 ibib hitstr abs

L1 ANSWER 1 OF 1 CAPLUS COPYRIGHT 2002 ACS
ACCESSION NUMBER: 1996:202911 CAPLUS
DOCUMENT NUMBER: 124:289981
TITLE: 2-(Hydroxyalkyl)estradiols: Synthesis and Biological
Evaluation
AUTHOR(S): Lovely, Carl J.; Gilbert, Nancy E.; Liberto, Muriel
M.; Sharp, Damon W.; Lin, Young C.; Brueggemeier,
Robert W.
CORPORATE SOURCE: Division of Medicinal Chemistry and Pharmacognosy,
College of Pharmacy, Columbus, OH, 43210, USA
SOURCE: Journal of Medicinal Chemistry (1996), 39(9), 1917-23
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



AB Synthetic estrogens possessing hydroxyalkyl side chains at the C-2 position of the A-ring were designed in order to further elucidate the structural and electronic requirements of the estrogen receptor to A-ring modifications. Furthermore, these compds. were envisaged as being stable analogs of the estradiol metabolite 2-hydroxyestradiol. The homologous series of 2-(hydroxyalkyl)estradiols I [R = (CH₂)_nOH, n = 1 - 3] has been prepd. by chain extension of 2-formylestradiol I (R = CHO), which, in turn, was prepd. via ortholithiation of estradiol. The substituted estradiols I [R = (CH₂)_nOH, n = 1 - 3] were assayed for their abilities to bind to the estrogen receptor in MCF-7 cells and induce estrogen-responsive gene expression. The estradiol homologs exhibited significantly weaker affinity than estradiol for the MCF-7 cell estrogen receptor, with relative binding affinities (estradiol = 100) ranging from 1.11 for 2-(hydroxymethyl)estradiol (I; R = CH₂OH) to 0.073 for 2-(hydroxypropyl)estradiol (I; R = CH₂CH₂CH₂OH). The relative activities for mRNA induction of the pS2 gene by the estradiol homologs closely parallel the relative binding affinities for the estrogen receptor in MCF-7 cells. 2-(Hydroxymethyl)estradiol (I; R = CH₂OH) exhibited similar estrogen receptor affinity and pS2 gene induction to the catechol estrogen 2-hydroxyestradiol and may prove useful in examn. of the further biol. effects of 2-hydroxyestrogen homologs.

=> s estradiol

11/30/02